10/538,998 YONG CHU 6-12-2006

$%^STN;HighlightOn=;**HighlightOff=**;

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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 4	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS 5	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS 6	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS 7	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS 8	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 9	MAR 22	EMBASE is now updated on a daily basis
NEWS 10	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 11	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS 12	APR 04	STN AnaVist $500 visualization usage credit offered
NEWS 13	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 14	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS 15	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS 16	MAY 10	CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS 17	MAY 11	KOREAPAT updates resume
NEWS 18	MAY 19	Derwent World Patents Index to be reloaded and enhanced
NEWS 19	MAY 30	IPC 8 Rolled-up Core codes added to CA/CAplus and USPATFULL/USPAT2
NEWS 20	MAY 30	The F-Term thesaurus is now available in CA/CAplus
NEWS 21	JUN 02	The first reclassification of IPC codes now complete in INPADOC
NEWS EXPRESS		FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/
NEWS HOURS		STN Operating Hours Plus Help Desk Availability
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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:56:24 ON 12 JUN 2006

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 12:56:37 ON 12 JUN 2006
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STRUCTURE FILE UPDATES: 11 JUN 2006 HIGHEST RN 887399-72-6
DICTIONARY FILE UPDATES: 11 JUN 2006 HIGHEST RN 887399-72-6

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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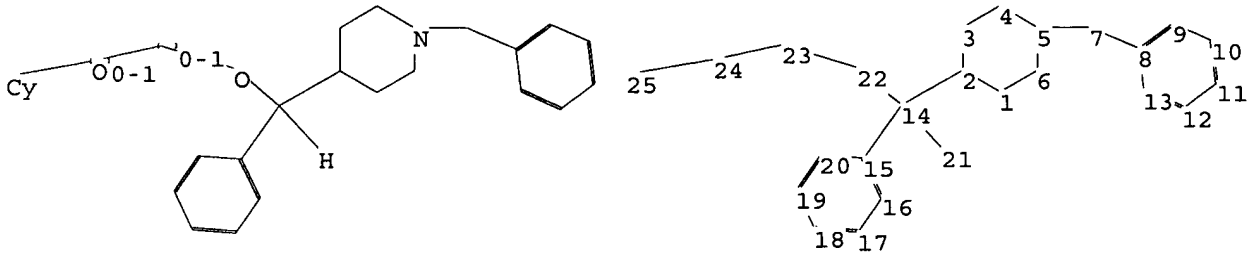
Uploading C:\Program Files\Stnexp\Queries\10538998\10538998f.str



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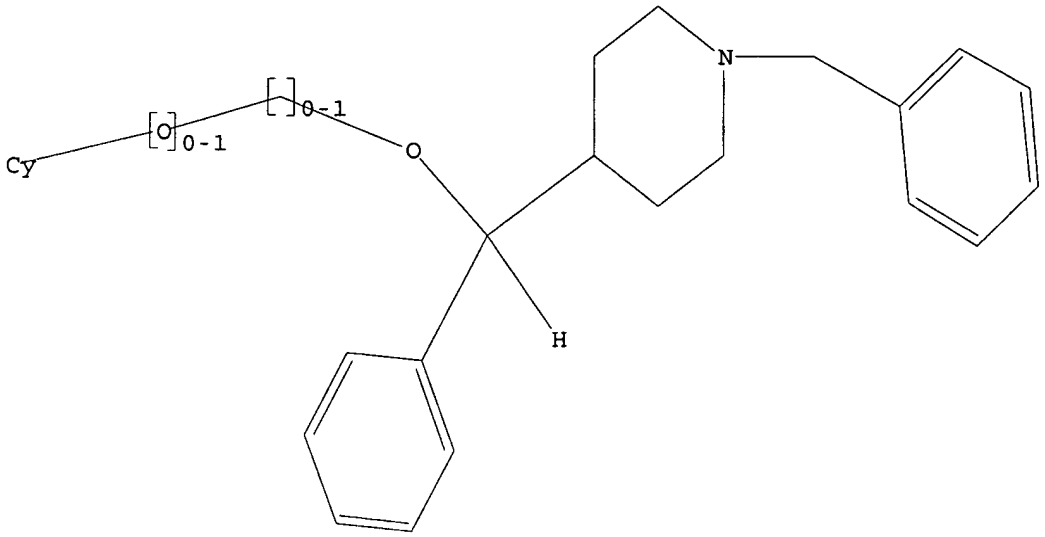
7 14 21 22 23 24 25
ring nodes :
1 2 3 4 5 6 8 9 10 11 12 13 15 16 17 18 19 20
chain bonds :
2-14 5-7 7-8 14-15 14-21 14-22 22-23 23-24 24-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-20
16-17 17-18 18-19 19-20
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 14-22 22-23 23-24 24-25
exact bonds :
2-14 7-8 14-15 14-21
normalized bonds :
8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-20 16-17 17-18 18-19 19-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:Atom
Generic attributes :
25:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 12:56:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      771 TO ITERATE

100.0% PROCESSED      771 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        13755 TO    17085
PROJECTED ANSWERS:               3 TO      163

L2            3 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 12:57:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    15300 TO ITERATE

100.0% PROCESSED    15300 ITERATIONS                               25 ANSWERS
SEARCH TIME: 00.00.01

L3           25 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   166.94     167.15

FILE 'CAPLUS' ENTERED AT 12:57:12 ON 12 JUN 2006
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FILE COVERS 1907 - 12 Jun 2006 VOL 144 ISS 25
FILE LAST UPDATED: 11 Jun 2006 (20060611/ED)

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=> s l3
L4 3 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:589417 CAPLUS
DOCUMENT NUMBER: 141:140320
TITLE: A preparation of insecticidal piperidine and pyridine derivatives
INVENTOR(S): Ding, Ping; Henrie, Robert H., II; Cohen, Daniel H.; Lyga, John W.; Rosen, David S.; Theodoridis, George; Zhang, Qun; Yeager, Walter H.; Donovan, Stephen F.; Zhang, Steven Shunxiang; Shulman, Inna; Yu, Seong Jae; Wang, Guozhi; Zhang, Y. Larry; Gopalsamy, Ariamala; Warkentin, Dennis L.; Rensner, Paul E.; Silverman, Ian R.; Cullen, Thomas G.
PATENT ASSIGNEE(S): FMC Corporation, USA
SOURCE: PCT Int. Appl., 182 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

Current appl.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004060371	A1	20040722	WO 2003-US38878	20031208
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003296308	A1	20040729	AU 2003-296308	20031208
EP 1572207	A1	20050914	EP 2003-814662	20031208
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003017324	A	20051116	BR 2003-17324	20031208
CN 1729178	A	20060201	CN 2003-80106750	20031208
CN 1744895	A	20060308	CN 2003-80109445	20031208
PRIORITY APPLN. INFO.:			US 2003-495059P P	20030814
			WO 2003-US38878 W	20031208

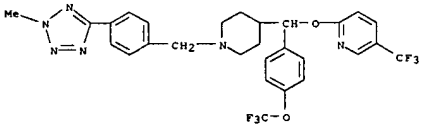
OTHER SOURCE(S): MARPAT 141:140320
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

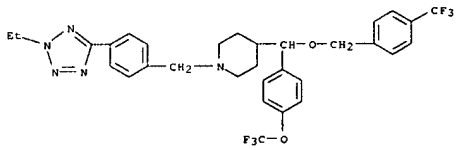
AB The invention relates to a preparation of insecticidal piperidine and pyridine derivs. of formula I [wherein: A is C or CH; B is substituted phenyl; C is O-1; D is (CH2)0-3; E is a bridging group selected from (CR9R10)-(CR11R12)0-1, (CR9R10)-(CR11R12)0-1O, C3H6, C(O), or C(S)NH, etc.; R1 is H, alkyl, alkoxyalkyl, or aryl; R2, R3, R4, R5, and R6 are independently selected from H, halogen, (halo/hydroxy)alkyl, alkylthio, CN, or NO2, etc.; R7 is (halo/hydroxy/alkoxy/dialkylamino)alkyl, sulfonatoalkyl, arylalkyl, or arylcarbonyl, etc.; R8 is H, (cyclo)alkyl, alkoxy, amino, morpholinyl, or indolyl, etc.; R9, R10, R11, and R12 are independently selected from H, alkyl, aryl, etc.]. Prepd. compds. were evaluated for activity against tobacco budworm in a surface-treated diet test. For instance, piperidine deriv. II (compd. 101, insecticidal activity: 100% mortality, 100% growth inhibition) was prepd. via elimination reaction of hydroxymethylpiperidine deriv. III, N-benzylation of the obtained methylenepiperidine deriv. IV by 4-nitrophenylmethyl bromide, subsequent redn. of the nitro-group, N-carboxylation of the obtained amine V, and N-oxidn. (example 1).

IT **726127-41-9P 726129-23-3P 726129-24-4P**
726129-25-5P 726129-26-6P 726129-27-7P
726129-92-6P 726129-94-8P 726129-95-9P
726129-97-1P 726129-98-2P 726129-99-3P
726130-00-3P 726130-08-1P 726130-09-2P
726130-10-5P 726130-11-6P 726130-12-7P
726130-13-8P 726132-15-6P 726133-18-2P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of insecticidal piperidine and pyridine derivs.)

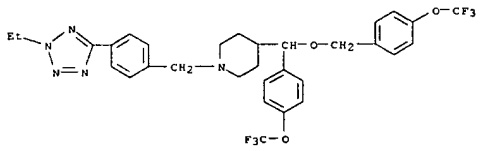
RN 726127-41-9 CAPLUS
CN Pyridine, 2-[[1-[[4-(2-methyl-2H-tetrazol-5-yl)phenyl]methyl]-4-piperidinyl][4-(trifluoromethoxy)phenyl]methoxy]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



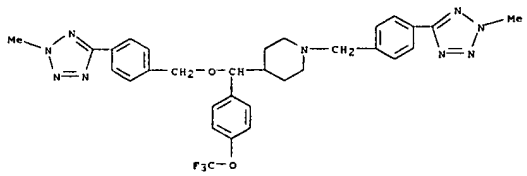
RN 726129-23-3 CAPLUS
CN Piperidine, 1-[[4-(2-ethyl-2H-tetrazol-5-yl)phenyl]methyl]-4-[[4-(trifluoromethoxy)phenyl][[4-(trifluoromethyl)phenyl]methoxy]methyl]- (9CI) (CA INDEX NAME)



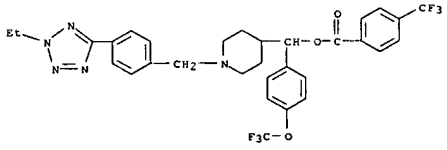
RN 726129-24-4 CAPLUS
CN Piperidine, 1-[[4-(2-ethyl-2H-tetrazol-5-yl)phenyl]methyl]-4-[[4-(trifluoromethoxy)phenyl][[4-(trifluoromethoxy)phenyl]methoxy]methyl]- (9CI) (CA INDEX NAME)



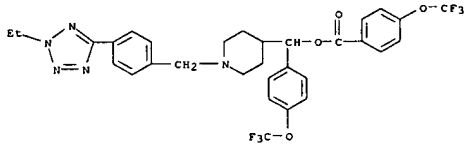
RN 726129-25-5 CAPLUS
CN Piperidine, 4-[[[4-(2-methyl-2H-tetrazol-5-yl)phenyl]methoxy][4-(trifluoromethoxy)phenyl]methyl]-1-[[4-(2-methyl-2H-tetrazol-5-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)



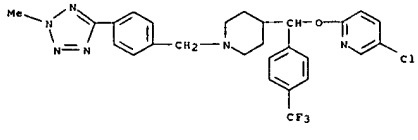
RN 726129-26-6 CAPLUS
CN Benzoic acid, 4-(trifluoromethyl)-, [1-[[4-(2-ethyl-2H-tetrazol-5-yl)phenyl]methyl]-4-piperidinyl][4-(trifluoromethoxy)phenyl]methyl ester (9CI) (CA INDEX NAME)



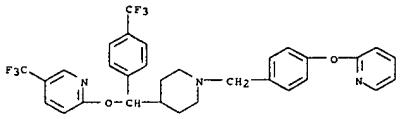
RN 726129-27-7 CAPLUS
CN Benzoic acid, 4-(trifluoromethoxy)-, [1-[[4-(2-ethyl-2H-tetrazol-5-yl)phenyl]methyl]-4-piperidinyl][4-(trifluoromethoxy)phenyl]methyl ester (9CI) (CA INDEX NAME)



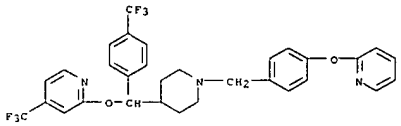
RN 726129-92-6 CAPLUS
CN Pyridine, 5-chloro-2-[[1-[[4-(2-methyl-2H-tetrazol-5-yl)phenyl]methyl]-4-piperidinyl][4-(trifluoromethyl)phenyl]methoxy]- (9CI) (CA INDEX NAME)



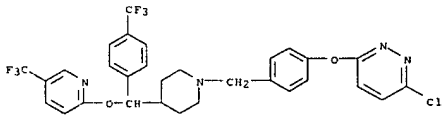
RN 726129-94-8 CAPLUS
CN Pyridine, 2-[[1-[[4-(2-pyridinyloxy)phenyl]methyl]-4-piperidinyl][4-(trifluoromethyl)phenyl]methoxy]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



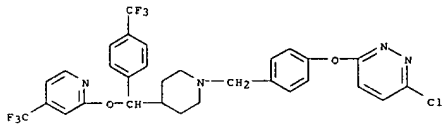
RN 726129-95-9 CAPLUS
CN Pyridine, 2-[[1-[[4-(2-pyridinyloxy)phenyl]methyl]-4-piperidinyl][4-(trifluoromethyl)phenyl]methoxy]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

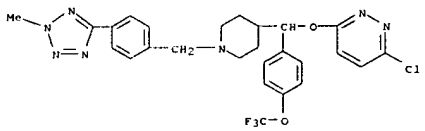


RN 726129-97-1 CAPLUS
CN Pyridazine, 3-chloro-6-[4-[[4-[[4-(trifluoromethyl)phenyl][[5-(trifluoromethyl)-2-pyridinyl]oxy]methyl]-1-piperidinyl]methyl]phenoxy]- (9CI) (CA INDEX NAME)

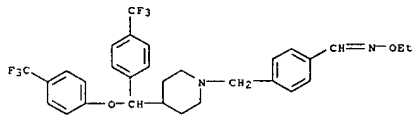


RN 726129-98-2 CAPLUS
CN Pyridazine, 3-chloro-6-[4-[[4-[[4-(trifluoromethyl)phenyl][[4-(trifluoromethyl)-2-pyridinyl]oxy]methyl]-1-piperidinyl]methyl]phenoxy]- (9CI) (CA INDEX NAME)

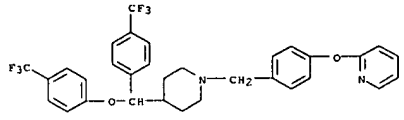




RN 726130-10-5 CAPLUS
CN Benzaldehyde, 4-[[4-[[4-(trifluoromethyl)phenoxy][4-(trifluoromethyl)phenyl]methyl]-1-piperidinyl]methyl]-, O-ethyloxime (9CI) (CA INDEX NAME)

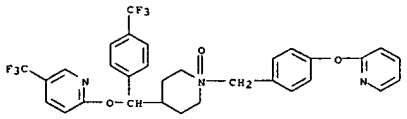


RN 726130-11-6 CAPLUS
CN Pyridine, 2-[4-[[4-[[4-(trifluoromethyl)phenoxy][4-(trifluoromethyl)phenyl]methyl]-1-piperidinyl]methyl]phenoxy]- (9CI) (CA INDEX NAME)

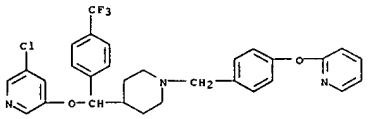


RN 726130-12-7 CAPLUS
CN Pyrimidine, 2-[4-[[4-[[4-(trifluoromethoxy)phenyl][4-(trifluoromethyl)phenoxy]methyl]-1-piperidinyl]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 726129-99-3 CAPLUS
CN Pyridine, 2-[[1-oxido-1-[[4-(2-pyridinyloxy)phenyl]methyl]-4-piperidinyl][4-(trifluoromethyl)phenyl]methoxy]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 726130-00-3 CAPLUS
CN Pyridine, 3-chloro-5-[[1-[[4-(2-pyridinyloxy)phenyl]methyl]-4-piperidinyl][4-(trifluoromethyl)phenyl]methoxy]- (9CI) (CA INDEX NAME)



RN 726130-08-1 CAPLUS
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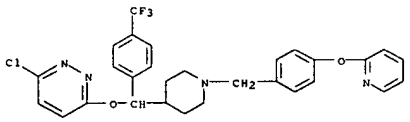
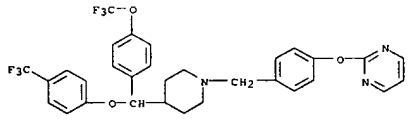
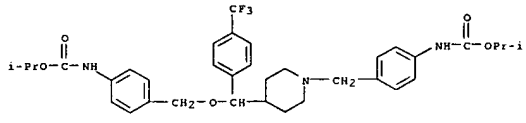


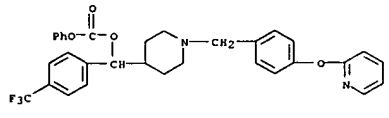
RN 726130-09-2 CAPLUS
CN Pyridazine, 3-chloro-6-[[1-[[4-(2-methyl-2H-tetrazol-5-yl)phenyl]methyl]-4-piperidinyl][4-(trifluoromethoxy)phenyl]methoxy]- (9CI) (CA INDEX NAME)



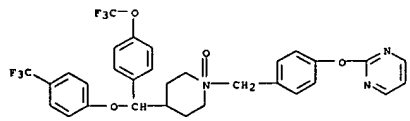
RN 726130-13-8 CAPLUS
CN Carbamic acid, [4-[[4-[[[4-[[(1-methylethoxy)carbonyl]amino]phenyl]methoxy][4-(trifluoromethyl)phenyl]methyl]-1-piperidinyl]methyl]phenyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)



RN 726132-15-6 CAPLUS
CN Carbonic acid, phenyl [1-[[4-(2-pyridinyloxy)phenyl]methyl]-4-piperidinyl][4-(trifluoromethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)



RN 726133-18-2 CAPLUS
CN Pyrimidine, 2-[4-[[1-oxido-4-[[4-(trifluoromethoxy)phenyl][4-(trifluoromethyl)phenoxy]methyl]-1-piperidinyl]methyl]phenoxy]- (9CI) (CA INDEX NAME)



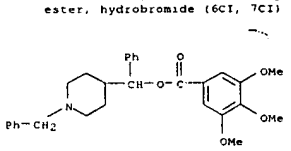
L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1-benzyl-4-piperidyl, H, H, H, H, MeO, MeO, MeO, H, --, --[HBr salt m. 227-30° (abs. EtOH-ether)]; O, O, 4-pyridyl, H, H, H, CO2H, H, H, H, H, .apprx.201-2°, --; O, O, 4-pyridyl, H, H, H, CO2Me, H, H, H, --, 96-9°; O, O, 4-pyridyl, H, H, H, H, H, CO2Et, H, H, --, --, O, O, 4-pyridyl, H, H, H, NO2, H, H, H, H, --, --; O, O, 4-pyridyl, H, H, H, H, H, NO2, H, H, --, 224-7°; O, O, 4-pyridyl, H, H, H, H, NMe2, H, H, H, --(b0.2 200-10°), --; O, O, 4-pyridyl, H, H, H, H, H, NEt2, H, H, --, --. Also prepd. were the following (m.p. and m.p. HCl salt given): α-phenyl-4-pyridinemethyl 3,4,5-trimethoxycinnamate, --, 200-1°; α-phenyl-4-pyridinemethyl 3,4,5-trimethoxybenzoate N-oxide, --, --(λ 6.72 μ); 4-pyridinemethyl 3,3,5-trimethoxybenzoate, -, 210-11° (EtOH); α,α-diphenyl-4-pyridinemethyl 3,4,5-trimethoxybenzoate, 160.5-1.5° (iso-PrOH), --. Also prepd. are (m.p. given): (3,4,5-Cl3C6H2CO)2O, 206-10°; α-m-tolyl-4-pyridinemethanol, 147-50° (C6H6); α-m-chlorophenyl-4-pyridinemethanol, 133-5°; α-phenyl-4-piperidinemethanol, 168-9° (abs. EtOH); 4-benzoyl-1-methylpyridinium iodide, --; 1-methyl-α-phenyl-4-piperidinemethanol, --; 4-benzoyl-1-benzylpyridinum chloride, .apprx.193-4° (butanone); 1-benzyl-α-phenyl-4-piperidinemethanol-HCl, 190-3° (abs. EtOH-anhyd. ether).

IT **98023-55-3**, 4-Piperidinemethanol, 1-benzyl-α-phenyl-, 3,4,5-trimethoxybenzoate, hydrobromide
(preparation of)

RN 98023-55-3 CAPLUS

CN Benzoic acid, 3,4,5-trimethoxy-, α-(1-benzyl-4-piperidyl)benzyl ester, hydrobromide (6CI, 7CI) (CA INDEX NAME)



● HBr

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1954:28787 CAPLUS
DOCUMENT NUMBER: 48:28787
ORIGINAL REFERENCE NO.: 48:5189d-i,5190a-i,5191a-c
TITLE: Quinolyl ketones. I
AUTHOR(S): de Diesbach, Henri; Pugin, Andre; Morard, Francois; Nowaczinski, Wojceich; Dessibourg, Joseph
CORPORATE SOURCE: Univ. Fribourg, Switz.
SOURCE: Helvetica Chimica Acta (1952), 35, 2322-32
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 48:28787

GI For diagram(s), see printed CA Issue.

AB A number of quinolyl ketones (I), prepared by the Skraup synthesis from 4-aminobenzophenones, have been reduced with Raney Ni and H at ordinary pressure and temperature to the tetrahydro derivs. (II) and with (iso-PrO)3Al to the carbinols (III), but could not be reduced to the tetrahydro carbinols (IV.). Raney Ni reduces III to the methylene derivs. (V) instead of to IV. Thus 6-benzoylquinoline (VI), colorless crystals, m. 60.5° (from ligroine) [VI.H2O, white plates, m. 39-40° (from MeOH or EtOH); picrate, m. 222°; phenylhydrazone, m. 184°; syn-oxime, m. 198-205°; anti-oxime, m. 192-5°], is prepared by heating p-H2NC6H4Bz, PhNO2, glycerol, and concentrated H2SO4 3 h. at 160°, diluting, treating with steam, acidifying, alkalizing, taking up in Et2O, filtering, and distilling at 240°/16 mm. Similarly are prepared the following compds. [(a) starting amine, and (b) corresponding quinoline derivative]: (a) 3,4-Me(H2N)C6H3Bz; (b) 6-benzoyl-8-methylquinoline. (VII), yellowish plates, m. 199° (from AcOH) [phenylhydrazone, m. 235-7° (from C6H6)]. (a) 4-Amino-4'-chlorobenzophenone; (b) 6-(p-chlorobenzoyl)quinoline (VIII), m. 204° (from ligroine, b. 120-80°, then from MeOH). (a) 4-Amino-2',4'-dichlorobenzophenone, m. 130-1° (100% yield by Raney Ni hydrogenation of the 4-nitro analog in MeOH 24 h. at 100° and 80 atmospheric); (b) 6-(2,4-dichlorobenzoyl)quinoline (IX), white crystals, m. 131-2°. (a) 4-Amino-2',5'-dichlorobenzophenone, white crystals, m. 123° (from 60% alc.), from the 4-nitro analog with SnCl2 or Na2S; (b) 6-(2,5-dichlorobenzoyl)quinoline (X), white needles, m. 134-5° (from dilute alc.) (picrate, m. 208-9°). (a) 4-Amino-3',4'-dichlorobenzophenone, white crystals, m. 161-2° (from alc.), from the 4-nitro compound with SnCl2; (b) 6-(3,4-dichlorobenzoyl)quinoline (XI), m. 139-40° (from ligroine and MeOH) (picrate, m. 173-4°). (a) 4-Amino-4'-chlorobenzophenone; (b) 6-(4-chlorobenzyl)quinoline, m. 191.5-2° (from alc.). (a) 4-Amino-2',4'-dichlorodiphenylmethane, blue crystals, m. 102-3° (Ac derivative, m. 141-2°), from the 4-nitro compound with SnCl2; (b) 6-(2,4-dichlorobenzyl)quinoline (in poor yield) (picrate, m. 167-8°). (a) 4-Amino-3',4'-dichlorodiphenylmethane, an oil (Bz derivative, m. 106-7°), from the 4-nitro compound and SnCl2; (b) 6-(3,4-dichlorobenzyl)quinoline (picrate, m. 164-5°). 6-Acetyl-1,2,3,4-tetrahydroquinoline (XII), greenish plates, m. 105-7° (picrate, m. 125°; oxime, m. 144°), is prepared by condensing 1-acetyl-1,2,3,4-tetrahydroquinoline with ClCH2COCl at room temperature, saponifying the 1-Ac group with boiling 20% HCl, and heating in 80% alc. with powdered Fe and 2N HCl; heated 5 h. at 186° in a sealed tube with Hg(OAc)2, AcOH, and H2O it gives yellowish prisms of

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1964:16612 CAPLUS
DOCUMENT NUMBER: 60:16612
ORIGINAL REFERENCE NO.: 60:2903b-h
TITLE: Phenyl(pyridyl or piperidyl)alkyl benzoates and phenylalkanoates
INVENTOR(S): Rorig, Kurt J.
PATENT ASSIGNEE(S): G.D. Searle and Co.
SOURCE: 10 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3100775		19630813	US 1959-803371	19590401

GI For diagram(s), see printed CA Issue.

AB Carbinols of the general formula RR'ArCR''nOH, where R is an alkyl or aryl group, R' is a pyridyl or piperidyl group, Ar is an aryl group, R'' is an alkylene group, and n is 0 or 1, are treated with anhydrides of the general formula (PhRnCO)2O, where R is an alkylene group and n is 0 or 1, to give the title compds. which can be used as spasmolytic and fungicidal agents. Thus, a mixture of α-phenyl-4-pyridinemethanol 25 and o-ClC6H4COCl 60 parts is heated 11 hrs. under N at 130-50°, cooled to .apprx.30°, treated with excess 10% NaOH, and extracted with ether. The ether extract is extracted with dilute HCl, the acid extract made alkaline with NaOH, the precipitate separated and taken up in ether, the ether mixture filtered, dried, and evaporated, and the residue obtained distilled in vacuo to give α-phenyl-4-pyridylmethyl o-chlorobenzoate, b0.15 175-95°. Similarly prepared are the following I (m, n, R, R1, R2, R3, X, X1, X2, X3, X4, m.p., and m.p. HCl salt given): 0, 0, 4-pyridyl, H,H,H, H, H, Cl, H, H, .apprx.68-9° (petr. ether), --; 0, 0, 2-pyridyl, H, H, H, H, H, Cl, H, H, .apprx.76-7° (petr. ether), --; 0, 0, 4-pyridyl, H, H, H, H, Cl, Cl, Cl, H, --, 205-7° (EtOH-ether); 0, 0, 4-pyridyl, H, H, H, MeO, H, H, H, H, --(b0.8 180-215°), --; 0, 0, 4-pyridyl, H, H, H, H, H, MeO, H, H, 94-6° (b0.3 185-205°), --; 0, 0, 4-pyridyl, H, H, H, H, H, EtO, H, H, 96-9° (b0.3 195-200°), --; 0, 1, 4-pyridyl, H, H, H, H, H, MeO, H, H, --(b0.4 185-215°), --; 0, 0, 4-pyridyl, H, H, H, H, MeO, MeO, H, H, --, 210-12°; 0, 0, 4-pyridyl, H, H, H, H, MeO, MeO, MeO, H, 118-20°, .apprx.219-20° (EtOH-anhydrous ether) (maleate m. 117-19°); 0, 0,4-pyridyl, H, H, H, MeO, MeO, MeO, H, H, --, --; 0, 0, 4-pyridyl, H, H, H, MeO, H, MeO, H, MeO, --, --; 0, 0, 4-pyridyl, H, H, H, H, MeO, MeO, MeO, H, --, 202-4°; 0, 0, 2-pyridyl, H, H, H, H, MeO, MeO, MeO, H, 115-16° (iso-PrOH), 172.5.4° (EtOH-ether); 0, 0, 3-pyridyl, H, H, H, H, MeO, MeO, MeO, H, --, 192-4° (EtOH); 1, 0, 4-pyridyl, H, H, H, H, MeO, MeO, MeO, H, --, --; 2, 0, 4-pyridyl, H, H, H, H, MeO, MeO, MeO, H, --, --; 0, 1, 4-pyridyl, H, H, H, H, H, MeO, MeO, MeO, H, --, 182°; 0, 2, 4-pyridyl, H, H, H, H, MeO, MeO, MeO, H, --, --; 0, 0, 4-pyridyl, H, Me, H, H, MeO, MeO, MeO, H, --, 200-2° (absolute EtOH-ether); 0, 0, 4-pyridyl, H, Me, H, H, EtO, EtO, EtO, H, --, 207-10° (absolute EtOH); 0, 0, 4-pyridyl, H, H, Et, H, EtO, EtO, EtO, H, --, --; 0, 0, 4-pyridyl, H, Cl, H, H, MeO, MeO, MeO, H, --, 204-6° (absolute EtOH); 0, 0, 4-pyridyl, Cl, H, H, H, EtO, EtO, EtO, H, --, --; 0, 0, 4-piperidyl, H, H, H, H, MeO, MeO, MeO, H, --, --; 0, 0, 1-methyl-4-piperidyl, H, H, H, H, MeO, MeO, MeO, H, --, --; 0, 0, 1-octyl-4-piperidyl, H, H, H, H, MeO, MeO, MeO, H, --, --; 0, 0,

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

6-acetylquinoline, m. 75-6° (picrate, m. 242°). A Beckmann rearrangement of XII oxime gives 6-amino-1,2,3,4-tetrahydroquinoline, m. 95.5-6°. Na redn. of Quinaldine in AmOH gives 93% 1,2,3,4-tetrahydroquinaldine, acetylated with Ac2O to the 1-Ac deriv.,

b12

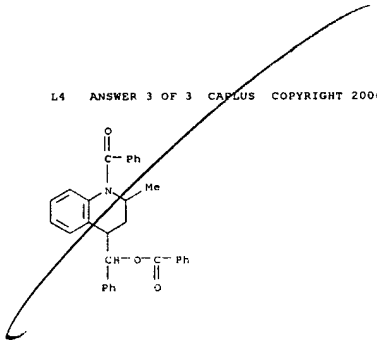
153°, yellow crystals, m. 57°; which, treated with ClCH2COCl in CS2, then slowly with AlCl3, and let stand 2 days yields 6-(chloroacetyl)-1,2,3,4-tetrahydroquinaldine-HCl, white crystals, m. 225-6°, converted by neutralization with dil. alkali to the free quinaldine, yellow crystals, m. 121°, which is dechlorinated in 80% HCl with Fe and 2N HCl to 6-acetyl-1,2,3,4-tetrahydroquinaldine, m. 69°. The following 1,2,3,4-tetrahydroquinolines are prepd. in good yield by hydrogenating 5 g. of the appropriate I in 50 mL. MeOH at room temp. and pressure in the presence of Raney Ni, warming, filtering, washing the Ni with warm MeOH, evapg. to a small vol., and recrystg.: 6-benzoyl (XIII), yellowish crystals, m. 113° [1-ON deriv., m. 119-20°; 1-Bz deriv., m. 131° (from 50% AcOH); 1-Ac deriv., m. 97° (from dil. alc.)]; 6-benzoyl-8-Me, pale yellow needles, m. 118°; 6-(p-chlorobenzoyl)tetrahydroquinoline, m. 156° (1-ON deriv., m. 173-4°; 6-Bz deriv., m. 146°); 6-(2,4-dichlorobenzoyl), m. 137° (1-ON deriv., m. 145°); 6-(2,5-dichlorobenzoyl), m. 153°. The Meerwein-Ponndorf redn. of I to III is carried out in nearly 100% yield by adding 10 g. of the I in 30 mL. iso-PrOH to (iso-PrO)3Al (made by refluxing 2.5 g. Al paste 10 h.

with

0.125 g. HgCl2 in 50 mL. abs. iso-PrOH), slowly distg. the Me2CO formed, alkalizing, steam-distg. the iso-PrOH, adding boiling H2O to the residue, and crystg. from dil. alc. Thus are prepd. the following carbinols: phenyl(6-quinolyl) (XIV), m. 127-8° (picrate, m. 190°; picrate of the acetate (ester), m. 188°); phenyl(8-methyl-6-quinolyl) (XV), m. 133° [picrate, m. 202-3°; acetate (ester), m. 100° (from dil. alc.)]; (p-chlorophenyl)(6-quinolyl), m. 153° (picrate, m. 186°; picrate of the acetate (ester), m. 209°); (2,4-dichlorophenyl)(6-quinolyl), m. 161° (picrate, m. 225°; acetate (ester), m. 125-6°; picrate of the acetate, m. 212°); X, (2, 5-dichlorophenyl)(6-quinolyl), m. 161° (acetate (ester), m. 174°); (3,4-dichlorophenyl)(6-quinolyl), m. 145° (picrate of the acetate (ester), m. 189-90°). Raney Ni hydrogenation of XIV gives 6-benzylquinoline, white crystals, m. 48-9°; similarly XV is reduced to 6-benzyl-8-methylquinoline, m. 55°. An attempted (iso-PrO)3Al redn. of XIII to the corresponding IV gives instead a white paste, m. 120-40°, sol. in C6H6 and CHCl3, slightly sol. in alc. 2-Benzoylquinoline is reduced by (iso-PrO)3Al in 100% yield to phenyl(2-quinolyl)carbinol (XVI), white crystals, m. 69° (from ligroine); also obtained by Raney Ni hydrogenation at room pressure and temp. [picrate, yellow crystals, m. 138° (from alc.)], instead of to the tetrahydro deriv. Phenyl(1,2,3,4-tetrahydro-2-quinalyl)carbinol, b0.005 140° [1-ON deriv., yellow plates, m. 103° (from dil. alc.); N,O-di-Bz deriv., m. 161° (from ligroine)], is prepd. by reducing 2 g. 2-benzoylquinoline 1 h. in 300 g. MeOH with H at 70° and 50 atm. in the presence of Raney Ni, filtering, washing with MeOH, evapg. to a small vol., dilg. with H2O, adding Et2O, and vacuum-distg.

the

oil. 4-Benzoylquinoline is reduced by (iso-PrO)3Al to phenyl(4-quinolyl)carbinol, m. 127° (from dil. alc.) (acetate (ester), white plates, m. 100°), and by Raney Ni hydrogenation at 100° and 70 atm. to phenyl(1,2,3,4-tetrahydro-4-quinolyl)carbinol, m. 135° (from dil. alc.), b0.001 110-15° [1-ON deriv., yellow leaves, m. 105° (from dil. ac.); N,O-di-Bz deriv., m.



L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

156° (from ligroine)]. 2-Methyl-4-benzoylquinoline (XVII), bright plates, m. 118° (from ligroine), is prepd. by heating 2 g. 2-methyl-4-quinolinecarboxamide in 30 mL. POCl3 with 3 g. PCl5 (with 2 drops water added to start the reaction) 15-20 min. at 110°, cooling with ice, neutralizing, extg. with Et2O, crystg. from ligroine

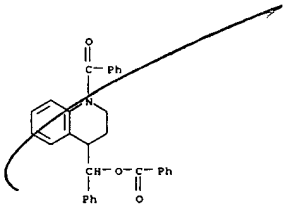
the

2-methyl-4-cyanoquinoline (XVIII), white needles, m. 106°, and adding the Grignard reagent from 12 g. PhBr and 2 g. Mg in 30 mL. Et2O to 5 g. XVIII in 50 mL. Et2O; XVII is reduced by (iso-Pr)3Al to phenyl(2-methyl-4-quinolyl)carbinol, colorless prisms, m. 167° (from dil. alc.) [acetate (ester), m. 103° (from dil. alc.)], and by Raney Ni hydrogenation at 100° and 70 atm. to phenyl(2-methyl-1,2,3,4-tetrahydro-4-quinolyl)carbinol, m. 162° (from dil. alc.), b0.001 130° [N,O-Bz deriv., m. 149° (from ligroine)]. Raney Ni redn. at room pressure and temp. of 8-benzoylquinoline gives at once phenyl(1,2 3,4-tetrahydro-8-quinolyl)carbinol, oil, b0.001 120° [1-ON deriv., yellow prisms, m. 146° (from alc.), (di-Bz deriv., m. 132° (from ligroine)]. Nitration of 6 g. VI in 25 mL. concd. H2SO4 with 1 mL. nitrating mixt. (= 0.255 g. HNO3) added at -10°, followed by cooling with ice, filtering, neutralizing with NH4OH, and crystg. in alc., gives 6-(m-nitrobenzoyl)quinoline, yellow needles, m. 160°, which reduced by SnCl2 in alc. to the amino compd., yellow crystals, m. 142° (from H2O). Similarly, VII is nitrated to 6-(m-nitrobenzoyl)-8-methylquinoline, m. 156°, which is reduced to the 3-amino compd., yellow crystals, m. 187° (from ligroine). The (dichlorobenzoyl)quinolines cannot be nitrated.

IT **858473-25-3**, 4-Quinolinemethanol, 1-benzoyl-1,2,3,4-tetrahydro-α-phenyl-, benzoate **858473-28-6**, 4-Quinolinemethanol, 1-benzoyl-1,2,3,4-tetrahydro-2-methyl-α-phenyl-, benzoate (preparation of)

RN 858473-25-3 CAPLUS

CN 4-Quinolinemethanol, 1-benzoyl-1,2,3,4-tetrahydro-α-phenyl-, benzoate (5CI) (CA INDEX NAME)



RN 858473-28-6 CAPLUS

CN 4-Quinolinemethanol, 1-benzoyl-1,2,3,4-tetrahydro-2-methyl-α-phenyl-, benzoate (5CI) (CA INDEX NAME)

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---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	15.79	182.94

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.25	-2.25

STN INTERNATIONAL LOGOFF AT 12:57:50 ON 12 JUN 2006